Roberto Improta

List of Publications by Year
in descending order

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217 papers	11,431 citations	30047 54 h-index	36008 97 g-index
227 all docs	227 docs citations	227 times ranked	6927 citing authors

#	Article	IF	Citations
1	A state-specific polarizable continuum model time dependent density functional theory method for excited state calculations in solution. Journal of Chemical Physics, 2006, 125, 054103.	1.2	675
2	Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzbergâ€“Teller effect: The Qx band of porphyrin as a case study. Journal of Chemical Physics, 2008, 128, 224311.	1.2	523
3	Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. Journal of Chemical Physics, 2007, 126, 084509.	1.2	445
4	Toward effective and reliable fluorescence energies in solution by a new state specific polarizable continuum model time dependent density functional theory approach. Journal of Chemical Physics, 2007, 127, 074504.	1.2	437
5	Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases. Chemical Reviews, 2016, 116, 3540-3593.	23.0	375
6	Singlet Excited-State Behavior of Uracil and Thymine in Aqueous Solution:Â A Combined Experimental and Computational Study of 11 Uracil Derivatives. Journal of the American Chemical Society, 2006, 128, 607-619.	6.6	359
7	Interplay of Electronic, Environmental, and Vibrational Effects in Determining the Hyperfine Coupling Constants of Organic Free Radicals. Chemical Reviews, 2004, 104, 1231-1254.	23.0	315
8	Effective method to compute vibrationally resolved optical spectra of large molecules at finite temperature in the gas phase and in solution. Journal of Chemical Physics, 2007, 126, 184102.	1.2	303
9	Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation. Journal of Chemical Theory and Computation, 2013, 9, 2072-2082.	2.3	194
10	Absorption and Fluorescence Spectra of Uracil in the Gas Phase and in Aqueous Solution:Â A TD-DFT Quantum Mechanical Study. Journal of the American Chemical Society, 2004, 126, 14320-14321.	6.6	181
11	DNA/RNA: Building Blocks of Life Under UV Irradiation. Journal of Physical Chemistry Letters, 2010, 1, 2025-2030.	2.1	177
12	Absolute pKa determination for carboxylic acids using density functional theory and the polarizable continuum model. Chemical Physics Letters, 2003, 373, 411-415.	1.2	173
13	Ab Initio Calculations of Absorption Spectra of Large Molecules in Solution: Coumarin C153. Angewandte Chemie - International Edition, 2007, 46, 405-408.	7.2	164
14	Quantum Mechanical Computations and Spectroscopy: From Small Rigid Molecules in the Gas Phase to Large Flexible Molecules in Solution. Accounts of Chemical Research, 2008, 41, 605-616.	7.6	155
15	Solvent Effect on the Singlet Excited-State Lifetimes of Nucleic Acid Bases:Â A Computational Study of 5-Fluorouracil and Uracil in Acetonitrile and Water. Journal of the American Chemical Society, 2006, 128, 16312-16322.	6.6	149
16	Electronic Excited States Responsible for Dimer Formation upon UV Absorption Directly by Thymine Strands: Joint Experimental and Theoretical Study. Journal of the American Chemical Society, 2012, 134, 14834-14845.	6.6	133
17	Understanding the Role of Stereoelectronic Effects in Determining Collagen Stability. 1. A Quantum Mechanical Study of Proline, Hydroxyproline, and Fluoroproline Dipeptide Analogues in Aqueous Solution. Journal of the American Chemical Society, 2001, 123, 12568-12577.	6.6	129
18	UV-Induced Proton Transfer between DNA Strands. Journal of the American Chemical Society, 2015, 137, 7059-7062.	6.6	125

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19	Influence of base stacking on excited-state behavior of polyadenine in water, based on time-dependent density functional calculations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9931-9936.	3.3	124
20	Structure and Conformational Behavior of Biopolymers by Density Functional Calculations Employing Periodic Boundary Conditions. I. The Case of Polyglycine, Polyalanine, and Poly-Î±-aminoisobutyric Acid in Vacuo. Journal of the American Chemical Society, 2001, 123, 3311-3322.	6.6	117
21	Photoinduced Dynamics of Guanosine Monophosphate in Water from Broad-Band Transient Absorption Spectroscopy and Quantum-Chemical Calculations. Journal of the American Chemical Society, 2009, 131, 5839-5850.	6.6	110
22	Parametrization and Validation of Intramolecular Force Fields Derived from DFT Calculations. Journal of Chemical Theory and Computation, 2007, 3, 1803-1817.	2.3	102
23	Excited States Decay of the Aâ˜T DNA: A PCM/TD-DFT Study in Aqueous Solution of the (9-Methyl-adenine)2Â·(1-methyl-thymine)2 Stacked Tetramer. Journal of the American Chemical Society, 2009, 131, 15232-15245.	6.6	101
24	Excited-State Behavior of trans and cis Isomers of Stilbene and Stiff Stilbene:Â A TD-DFT Study. Journal of Physical Chemistry A, 2005, 109, 10058-10067.	1.1	97
25	Singlet excited state dynamics of uracil and thymine derivatives: A femtosecond fluorescence upconversion study in acetonitrile. Chemical Physics Letters, 2006, 429, 551-557.	1.2	97
26	Checking the pH-Induced Conformational Transition of Prion Protein by Molecular Dynamics Simulations: Effect of Protonation of Histidine Residues. Biophysical Journal, 2004, 87, 3623-3632.	0.2	96
27	Computing the inhomogeneous broadening of electronic transitions in solution: a first-principle quantum mechanical approach. Physical Chemistry Chemical Physics, 2011, 13, 17007.	1.3	89
28	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. Physical Chemistry Chemical Physics, 2013, 15, 3736.	1.3	89
29	First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogenous broadening. Computational and Theoretical Chemistry, 2014, 1040-1041, 328-337.	1.1	88
30	The excited states of Ï€-stacked 9-methyladenine oligomers: a TD-DFT study in aqueous solution. Physical Chemistry Chemical Physics, 2008, 10, 2656.	1.3	86
31	Solvent Polarity and pH Effects on the Magnetic Properties of Ionizable Nitroxide Radicals:Â A Combined Computational and Experimental Study of 2,2,5,5-Tetramethyl-3-carboxypyrrolidine and 2,2,6,6-Tetramethyl-4-carboxypiperidine Nitroxides. Journal of Physical Chemistry A, 2002, 106, 10700-10706.	1.1	84
32	Quantum mechanical study of the conformational behavior of proline and 4R-hydroxyproline dipeptide analogues in vacuum and in aqueous solution. Journal of Computational Chemistry, 2002, 23, 341-350.	1.5	81
33	Absorption and Emission Spectra of a Flexible Dye in Solution: A Computational Time-Dependent Approach. Journal of Chemical Theory and Computation, 2013, 9, 4507-4516.	2.3	78
34	Interplay between â€œNeutralâ€•and â€œChargeâ€Transferâ€•Excimers Rules the Excited State Decay in Adenineâ€Rich Polynucleotides. Angewandte Chemie - International Edition, 2011, 50, 12016-12019.	7.2	76
35	Photophysics of Deoxycytidine and 5-Methyldeoxycytidine in Solution: A Comprehensive Picture by Quantum Mechanical Calculations and Femtosecond Fluorescence Spectroscopy. Journal of the American Chemical Society, 2017, 139, 7780-7791.	6.6	76
36	Solvent Effect on the Singlet Excited-state Dynamics of 5-Fluorouracil in Acetonitrile as Compared with Water. Journal of Physical Chemistry B, 2006, 110, 12843-12847.	1.2	75

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37	The Decay from the Dark nÏ€* Excited State in Uracil: An Integrated CASPT2/CASSCF and PCM/TD-DFT Study in the Gas Phase and in Water. Journal of Physical Chemistry B, 2008, 112, 10769-10772.	1.2	67
38	Understanding the Role of Stereoelectronic Effects in Determining Collagen Stability. 2. A Quantum Mechanical/Molecular Mechanical Study of (Proline-Proline-Glycine)n Polypeptides. Journal of the American Chemical Society, 2002, 124, 7857-7865.	6.6	66
39	Quantum Dynamics of the Ultrafast Ï€Ï€*/nÏ€* Population Transfer in Uracil and 5-Fluoro-Uracil in Water and Acetonitrile. Journal of Physical Chemistry B, 2009, 113, 14491-14503.	1.2	66
40	Vibrationally Resolved Absorption and Emission Spectra of Dithiophene in the Gas Phase and in Solution by First-Principle Quantum Mechanical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4483-4493.	2.3	66
41	Modeling Solvent Broadening on the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models. Journal of Chemical Theory and Computation, 2015, 11, 5810-5825.	2.3	66
42	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	64
43	Efficient UV-induced charge separation and recombination in an 8-oxoguanine-containing dinucleotide. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11612-11617.	3.3	64
44	Absorption of Low-Energy UV Radiation by Human Telomere G-Quadruplexes Generates Long-Lived Guanine Radical Cations. Journal of the American Chemical Society, 2017, 139, 10561-10568.	6.6	64
45	The polarizability in solution of tetra-phenyl-porphyrin derivatives in their excited electronic states: a PCM/TD-DFT study. Physical Chemistry Chemical Physics, 2009, 11, 4664.	1.3	61
46	Multiâ€Pathway Excited State Relaxation of Adenine Oligomers in Aqueous Solution: A Joint Theoretical and Experimental Study. Chemistry - A European Journal, 2013, 19, 3762-3774.	1.7	60
47	Resolving Ultrafast Photoinduced Deactivations in Water-Solvated Pyrimidine Nucleosides. Journal of Physical Chemistry Letters, 2017, 8, 1777-1783.	2.1	60
48	Can TDâ€DFT calculations accurately describe the excited states behavior of stacked nucleobases? The cytosine dimer as a test case. Journal of Computational Chemistry, 2008, 29, 957-964.	1.5	59
49	Accurate Steady-State and Zero-Time Fluorescence Spectra of Large Molecules in Solution by a First-Principle Computational Method. Journal of Physical Chemistry B, 2007, 111, 14080-14082.	1.2	58
50	Effect of C5-Methylation of Cytosine on the Photoreactivity of DNA: A Joint Experimental and Computational Study of TCG Trinucleotides. Journal of the American Chemical Society, 2014, 136, 10838-10841.	6.6	58
51	Radical cations of DNA bases: some insights on structure and fragmentation patterns by density functional methods. International Journal of Mass Spectrometry, 2000, 201, 321-336.	0.7	57
52	Vibronic Model for the Quantum Dynamical Study of the Competition between Bright and Charge-Transfer Excited States in Single-Strand Polynucleotides: The Adenine Dimer Case. Journal of Physical Chemistry A, 2009, 113, 15346-15354.	1.1	56
53	Assessing the reliability of density functional methods in the conformational study of polypeptides: The treatment of intraresidue nonbonding interactions. Journal of Computational Chemistry, 2004, 25, 1333-1341.	1.5	55
54	Solvent effects on electron-driven proton-transfer processes: adenineâ€“thymine base pairs. Physical Chemistry Chemical Physics, 2012, 14, 8981.	1.3	55

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55	Computation of protein pKâ€™s values by an integrated density functional theory/Polarizable Continuum Model approach. Theoretical Chemistry Accounts, 2004, 111, 237-245.	0.5	54
56	Excited State Proton Transfer Is Not Involved in the Ultrafast Deactivation of Guanineâ€“Cytosine Pair in Solution. Journal of the American Chemical Society, 2011, 133, 19664-19667.	6.6	54
57	Photophysics and Photochemistry of Thymine Deoxy-Dinucleotide in Water: A PCM/TD-DFT Quantum Mechanical Study. Journal of Physical Chemistry B, 2012, 116, 14261-14274.	1.2	54
58	The conformational behavior of polyglycine as predicted by a density functional model with periodic boundary conditions. Journal of Chemical Physics, 2001, 114, 2541-2549.	1.2	53
59	The excited states of adenine and thymine nucleoside and nucleotide in aqueous solution: a comparative study by time-dependent DFT calculations. Theoretical Chemistry Accounts, 2008, 120, 491-497.	0.5	50
60	Absorption and Emission Spectral Shapes of a Prototype Dye in Water by Combining Classical/Dynamical and Quantum/Static Approaches. Journal of Physical Chemistry A, 2015, 119, 5426-5438.	1.1	50
61	Adiabatic-Molecular Dynamics Generalized Vertical Hessian Approach: A Mixed Quantum Classical Method To Compute Electronic Spectra of Flexible Molecules in the Condensed Phase. Journal of Chemical Theory and Computation, 2020, 16, 1215-1231.	2.3	50
62	The excited electronic states of adenine-guanine stacked dimers in aqueous solution: a PCM/TD-DFT study. Physical Chemistry Chemical Physics, 2010, 12, 4934.	1.3	46
63	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. Physical Chemistry Chemical Physics, 2018, 20, 6877-6890.	1.3	46
64	Assessing the acidâ€“base and conformational properties of histidine residues in human prion protein (125â€“228) by means of pK a calculations and molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2006, 64, 167-177.	1.5	45
65	Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?. Journal of Chemical Theory and Computation, 2017, 13, 4636-4648.	2.3	45
66	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. Physical Chemistry Chemical Physics, 2010, 12, 10550.	1.3	43
67	The Interplay between Ï€Ï€*/nÏ€* Excited States in Gasâ€Phase Thymine: A Quantum Dynamical Study. ChemPhysChem, 2011, 12, 1957-1968.	1.0	43
68	Computational Design, Synthesis, and Mechanochromic Properties of New Thiopheneâ€Based Ï€â€Conjugated Chromophores. Chemistry - A European Journal, 2013, 19, 1996-2004.	1.7	43
69	A Theoretical Study on the Factors Influencing Cyanine Photoisomerization:Â The Case of Thiacyanine in Gas Phase and in Methanol. Journal of Chemical Theory and Computation, 2005, 1, 215-229.	2.3	42
70	Solvent Effects on the Steady-state Absorption and Fluorescence Spectra of Uracil, Thymine and 5-Fluorouracil. Photochemistry and Photobiology, 2007, 83, 595-599.	1.3	42
71	Cation Effect on the Electronic Excited States of Guanine Nanostructures Studied by Time-Resolved Fluorescence Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 14682-14689.	1.5	42
72	Quantum-classical effective-modes dynamics of the Ï€Ï€* â†' nÏ€* decay in 9H-adenine. A quadratic vibronic coupling model. Faraday Discussions, 2013, 163, 223.	1.6	42

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73	Polymerization Mechanism of Conjugated Dienes in the Presence of Zieglerâ˜Natta Type Catalysts:Â Theoretical Study of Butadiene and Isoprene Polymerization with CpTiCl3â˜MAO Initiator. Organometallics, 2000, 19, 411-419.	1.1	41
74	Time dependent DFT investigation on the two lowest 1Bu states of the trans isomer of stilbene and stiff-stilbenes. Chemical Physics Letters, 2004, 387, 509-516.	1.2	41
75	Computing the Absorption and Emission Spectra of 5-Methylcytidine in Different Solvents: A Test-Case for Different Solvation Models. Journal of Chemical Theory and Computation, 2016, 12, 4430-4439.	2.3	41
76	Multiple Electronic and Structural Factors Control Cyclobutane Pyrimidine Dimer and 6â€“4 Thymineâ€“Thymine Photodimerization in a DNA Duplex. Chemistry - A European Journal, 2017, 23, 15177-15188.	1.7	41
77	Excited-State Dynamics of DNA Duplexes with Different H-Bonding Motifs. Journal of Physical Chemistry Letters, 2016, 7, 950-954.	2.1	40
78	Peptide Bond Distortions from Planarity: New Insights from Quantum Mechanical Calculations and Peptide/Protein Crystal Structures. PLoS ONE, 2011, 6, e24533.	1.1	40
79	Quantum mechanical prediction of the magnetic titration curve of a nitroxide `spin probe'. Chemical Physics Letters, 2001, 336, 349-356.	1.2	39
80	Absorption Spectrum of Aâ€“T DNA Unraveled by Quantum Mechanical Calculations in Solution on the (dA)₂â‹…(dT)₂ Tetramer. ChemPhysChem, 2008, 9, 2531-2537.	1.0	39
81	Role of side chains in collagen triple helix stabilization and partner recognition. Journal of Peptide Science, 2009, 15, 131-140.	0.8	39
82	Optical Properties of Guanine Nanowires: Experimental and Theoretical Study. Journal of Physical Chemistry C, 2010, 114, 14339-14346.	1.5	39
83	A joint experimental/theoretical study of the ultrafast excited state deactivation of deoxyadenosine and 9-methyladenine in water and acetonitrile. Photochemical and Photobiological Sciences, 2013, 12, 1375-1386.	1.6	39
84	Excited States Behavior of Nucleobases in Solution: Insights from Computational Studies. Topics in Current Chemistry, 2014, 355, 329-357.	4.0	39
85	UV-induced damage to DNA: effect of cytosine methylation on pyrimidine dimerization. Signal Transduction and Targeted Therapy, 2017, 2, 17021.	7.1	39
86	Mechanism of Isoprene and Butadiene Polymerization in the Presence of CpTiCl3â˜MAO Initiator:Â A Theoretical Study. Macromolecules, 1997, 30, 2219-2227.	2.2	37
87	Structure and Magnetic Properties of Nitroxide Molecular Crystals by Density Functional Calculations Employing Periodic Boundary Conditions. Journal of the American Chemical Society, 2002, 124, 113-120.	6.6	37
88	Torsional Barriers and Correlations between Dihedrals inp-Polyphenyls. Journal of Physical Chemistry A, 2003, 107, 8665-8670.	1.1	37
89	Quantum Mechanical Calculations Unveil the Structure and Properties of the Absorbing and Emitting Excited Electronic States of Guanine Quadruplex. Chemistry - A European Journal, 2014, 20, 8106-8115.	1.7	37
90	Assessing solvent effects on the singlet excited state lifetime of uracil derivatives: A femtosecond fluorescence upconversion study in alcohols and D2O. Chemical Physics, 2008, 350, 186-192.	0.9	36

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91	Relative Stability of the L_a and L_b Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra. Journal of Physical Chemistry Letters, 2014, 5, 1806-1811.	2.1	36
92	Tautomers of a Fluorescent G Surrogate and Their Distinct Photophysics Provide Additional Information Channels. Angewandte Chemie - International Edition, 2016, 55, 7974-7978.	7.2	36
93	Conformational and Spectroscopic Analysis of the Tyrosyl Radical Dipeptide Analogue in the Gas Phase and in Aqueous Solution by a Density Functional/Continuum Solvent Model. Journal of the American Chemical Society, 2002, 124, 11531-11540.	6.6	35
94	PCM/TD-DFT study of the two lowest excited states of uracil derivatives in solution: The effect of the functional and of the cavity model. Computational and Theoretical Chemistry, 2009, 914, 87-93.	1.5	35
95	UV-Induced Adenine Radicals Induced in DNA A-Tracts: Spectral and Dynamical Characterization. Journal of Physical Chemistry Letters, 2016, 7, 3949-3953.	2.1	35
96	Ultrafast Dynamics of the Two Lowest Bright Excited States of Cytosine and 1-Methylcytosine: A Quantum Dynamical Study. Journal of Chemical Theory and Computation, 2020, 16, 5792-5808.	2.3	34
97	Contribution of dipoleâ€“dipole interactions to the stability of the collagen triple helix. Protein Science, 2008, 17, 955-961.	3.1	33
98	Conformational analysis of the tyrosine dipeptide analogue in the gas phase and in aqueous solution by a density functional/continuum solvent model. Journal of Computational Chemistry, 2002, 23, 650-661.	1.5	32
99	Barrierless photoisomerisation of the â€œsimplest cyanineâ€ Joining computational and femtosecond optical spectroscopies to trace the full reaction path. Physical Chemistry Chemical Physics, 2012, 14, 13350.	1.3	32
100	Effect of C5-Methylation of Cytosine on the UV-Induced Reactivity of Duplex DNA: Conformational and Electronic Factors. Journal of Physical Chemistry B, 2016, 120, 4232-4242.	1.2	32
101	Understanding Electron Transfer across Negatively-Charged Aib Oligopeptides. Journal of Physical Chemistry B, 2005, 109, 1023-1033.	1.2	31
102	Photoinduced Electron Transfer in DNA: Charge Shift Dynamics Between 8-Oxo-Guanine Anion and Adenine. Journal of Physical Chemistry B, 2015, 119, 7491-7502.	1.2	31
103	Adenine radicals generated in alternating AT duplexes by direct absorption of low-energy UV radiation. Faraday Discussions, 2018, 207, 181-197.	1.6	31
104	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The Ï€Ï€*/nÏ€* Decay of Thymine in Water as a Test Case. Journal of Chemical Theory and Computation, 2018, 14, 820-832.	2.3	31
105	Conformational Behavior of Macromolecules in Solution. Homopolypeptides of Î±-Aminoisobutyric Acid as Test Cases. Macromolecules, 2001, 34, 7550-7557.	2.2	30
106	Comprehensive Study of Guanine Excited State Relaxation and Photoreactivity in G-quadruplexes. Journal of Physical Chemistry Letters, 2019, 10, 6873-6877.	2.1	30
107	Stabilization of Mixed Frenkel-Charge Transfer Excitons Extended Across Both Strands of Guanineâ€“Cytosine DNA Duplexes. Journal of Physical Chemistry Letters, 2015, 6, 2247-2251.	2.1	29
108	Effective modeling of intrinsic and environmental effects on the structure and electron plaramagnetic resonance parameters of nitroxides by an integrated quantum mechanical/molecular mechanics/polarizable continuum model approach. Theoretical Chemistry Accounts, 2000, 104, 273-279.	0.5	28

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109	Femtosecond photoelectron spectroscopy of trans-stilbene above the reaction barrier. Chemical Physics, 2005, 310, 201-211.	0.9	28
110	Femtosecond study on the isomerization dynamics of NK88. I. Ground-state dynamics after photoexcitation. Journal of Chemical Physics, 2006, 125, 044512.	1.2	28
111	Femtosecond study on the isomerization dynamics of NK88. II. Excited-state dynamics. Journal of Chemical Physics, 2006, 125, 044513.	1.2	28
112	Conformational Behavior and Magnetic Properties of a Nitroxide Amino Acid Derivative in Vacuo and in Aqueous Solution. Journal of Physical Chemistry A, 2003, 107, 6264-6269.	1.1	27
113	On the controversial nature of the 1â€‰B1u and 2â€‰B1u states of trans-stilbene: The n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2009, 130, 174307.	1.2	27
114	Photoinduced long-lived charge transfer excited states in AT-DNA strands. Physical Chemistry Chemical Physics, 2016, 18, 21241-21245.	1.3	27
115	What Makes Thienoguanosine an Outstanding Fluorescent DNA Probe?. Journal of the American Chemical Society, 2020, 142, 16999-17014.	6.6	27
116	Does tetracycline bind helix 2 of prion? An integrated spectroscopical and computational study of the interaction between the antibiotic and Î± helix 2 human prion protein fragments. Proteins: Structure, Function and Bioinformatics, 2006, 66, 707-715.	1.5	26
117	Mode-specific vibrational relaxation of photoexcited guanosine 5â€²-monophosphate and its acid form: a femtosecond broadband mid-IR transient absorption and theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 1487-1499.	1.3	26
118	Development and Validation of Quantum Mechanically Derived Force-Fields: Thermodynamic, Structural, and Vibrational Properties of Aromatic Heterocycles. Journal of Chemical Theory and Computation, 2018, 14, 4884-4900.	2.3	26
119	The excited state behavior of cytosine in the gas phase: A TD-DFT study. Computational and Theoretical Chemistry, 2014, 1040-1041, 186-194.	1.1	25
120	Quantumâ€Classical Calculation of the Absorption and Emission Spectral Shapes of Oligothiophenes at Low and Room Temperature by Firstâ€Principle Calculations. ChemPhysChem, 2014, 15, 3320-3333.	1.0	25
121	Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
122	Unveiling Excited-State Chirality of Binaphthols by Femtosecond Circular Dichroism and Quantum Chemical Calculations. Journal of Physical Chemistry Letters, 2019, 10, 4089-4094.	2.1	25
123	Excited State Pathways Leading to Formation of Adenine Dimers. Journal of Physical Chemistry Letters, 2016, 7, 2020-2023.	2.1	24
124	Computation of Spectroscopic Parameters in vacuo and in Condensed Phases by Methods based on the Density Functional Theory. QSAR and Combinatorial Science, 2002, 21, 105-118.	1.4	23
125	Building cavities in a fluid of spherical or rod-like particles: A contribution to the solvation free energy in isotropic and anisotropic polarizable continuum model. Journal of Computational Chemistry, 2005, 26, 1096-1105.	1.5	23
126	Nonadiabatic Absorption Spectra and Ultrafast Dynamics of DNA and RNA Photoexcited Nucleobases. Molecules, 2021, 26, 1743.	1.7	23

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127	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. Physical Chemistry Chemical Physics, 2021, 23, 8181-8199.	1.3	22
128	Parametrization and Validation of Coarse Grained Force-Fields Derived from ab Initio Calculations. Journal of Chemical Theory and Computation, 2006, 2, 556-567.	2.3	21
129	The Peculiar Spectral Properties of Amino-Substituted Uracils: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry B, 2010, 114, 12708-12719.	1.2	21
130	TD-DFT Investigation of the Magnetic Circular Dichroism Spectra of Some Purine and Pyrimidine Bases of Nucleic Acids. Journal of Physical Chemistry A, 2015, 119, 5476-5489.	1.1	21
131	Specific Recognition of G-Quadruplexes Over Duplex-DNA by a Macromolecular NIR Two-Photon Fluorescent Probe. Journal of Physical Chemistry Letters, 2017, 8, 5915-5920.	2.1	21
132	Radicals generated in alternating guanineâ€“cytosine duplexes by direct absorption of low-energy UV radiation. Physical Chemistry Chemical Physics, 2018, 20, 21381-21389.	1.3	21
133	Radicals Generated in Tetramolecular Guanine Quadruplexes by Photoionization: Spectral and Dynamical Features. Journal of Physical Chemistry B, 2019, 123, 4950-4957.	1.2	21
134	Studying the excited electronic states of guanine rich DNA quadruples by quantum mechanical methods: main achievements and perspectives. Photochemical and Photobiological Sciences, 2020, 19, 436-444.	1.6	21
135	On the trade-off between processability and opto-electronic properties of single wall carbon nanotube derivatives in thin film heterojunctions. Journal of Materials Chemistry C, 2015, 3, 303-312.	2.7	20
136	Photoactivated proton coupled electron transfer in DNA: insights from quantum mechanical calculations. Faraday Discussions, 2018, 207, 199-216.	1.6	20
137	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. Chemical Physics, 2018, 515, 452-463.	0.9	19
138	Excitonic Model for Strongly Coupled Multichromophoric Systems: The Electronic Circular Dichroism Spectra of Guanine Quadruplexes as Test Cases. Journal of Chemical Theory and Computation, 2021, 17, 405-415.	2.3	19
139	Nucleic Acids as a Playground for the Computational Study of the Photophysics and Photochemistry of Multichromophore Assemblies. Accounts of Chemical Research, 2022, 55, 2077-2087.	7.6	19
140	Benzophenone Photophore Flexibility and Proximity: Molecular and Crystal-State Structure of a Bpa-Containing Trichogin Dodecapeptide Analogue. ChemBioChem, 2004, 5, 541-544.	1.3	18
141	Effect of amino substitution on the excited state dynamics of uracil. Photochemical and Photobiological Sciences, 2008, 7, 765-768.	1.6	18
142	Three-dimensional diabatic models for the Ï€Ï€*Ââ†' nÏ€* excited-state decay of uracil derivatives in solution. Theoretical Chemistry Accounts, 2009, 123, 273-286.	0.5	18
143	Potassium Ions Enhance Guanine Radical Generation upon Absorption of Low-Energy Photons by G-Quadruplexes and Modify Their Reactivity. Journal of Physical Chemistry Letters, 2020, 11, 1305-1309.	2.1	18
144	Adenine Radical Cation Formation by a Ligand-Centered Excited State of an Intercalated Chromium Polypyridyl Complex Leads to Enhanced DNA Photo-oxidation. Journal of the American Chemical Society, 2021, 143, 14766-14779.	6.6	18

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